

- $A_n$  cross-ring cleavage, in glycoconjugate mixtures, 1863  
Acetate-anion complex, monopositive, intrinsic hydration of, 777  
Acetonitrile, Ni(II) complex ion reactions with, in gas phase, 1128  
Acid(s), bitter, in hop extract, LC-APCI-MS of, 180  
Acidic heteroxylans, uronosyl substitution patterns in, ESI-MS/MS of, 43  
Acute myeloid leukemia, histone modifications in, HPLC and MS of, 77  
Acylphosphatidylglycerols, from *Salmonella typhimurium*, ESI-MS/MS of, 1  
Acylpolyamides, from spider venom, MS/MS of, 1636  
 $\alpha$ -Adducts, anionic, in gas phase, using electrospray ion source as chemical reactor, 927  
Adipocytes, free fatty acid transport in, multi imaging MS of, 1572  
Advanced glycation end products/peptides, enzymatic digestion and MS studies of, 496  
Affinity chromatography, in phosphopeptide quantification, 363  
Affinity probes, for peptides and proteins, carbon nanotubes as, in MALDI MS, 1629  
Affinity purified cross-linked peptides, MS detection of, 832  
Air, electrospraying water in, at atmospheric pressure, 253  
Alcohol consumption, ethyl sulfate as marker of, by LC-ESI-MS-MS, 1644  
Aliphatic phosphopeptides, dissociation of, ESI-FTICR-MS and IRMPD of, 121  
Alkali-metal ions, cleavage reactions of, positive ion ESI-MS/MS of, 689  
Alkenamides, fragmentation of, by collisional activation in triple quadrupole mass spectrometer, 1462  
Alkenones, polyunsaturated long chain, double bond location in, GC-MS in derivatization for, 1161  
Alkyl diselenide, mass spectra of, 1325  
Amide bond cleavage mechanism, of protonated oligopeptides, MS/MS of, 103  
Amide hydrogen/deuterium exchange, modeling data from, in protein-ligand interactions, 388  
Amine-trifluoroacetic acid self-assembly, 356  
Amines, isomeric arylglycoside gas phase reactivity toward, 244  
Amino acid(s)  
    in probing structure of cytochrome *c* by ESI-MS, 1612  
    single, distinguished in protein and tertiary structure probed by ECD, 1087  
Aminonitropyrene, LC-MS/MS analysis of, 1853  
Ammonia, elimination in condensation reactions in protonated dipeptides, 1025  
Ammonia radical cation, water-solvated, reactions with carbonyl compounds, 966  
AMPPNP, ESI-TOF-MS of, 1392  
Amyloid precursor proteins, potential cleavage sites of, LC-MS/MS of, 1780  
Angiotensin-converting enzyme (ACE) inhibitors, MS fragmentation of, 1300  
Anionic  $\alpha$ -adducts, in gas phase, using electrospray ion source as chemical reactor, 927  
Antioxidants, predicting activity of, 848  
Arginine, molecular recognition by anionic salt, 616  
Arginine-aldehyde adducts, in cytochrome *c* modification by 4-hydroxy-2-nonenal, 1136  
Arginine dipeptide isomers, discrimination of, ESI-ion trap MS and kinetic method for, 840  
Aromatic compounds, polycyclic, analysis with APCI-MS, charge exchange and proton transfer in, 301  
Aromatic phosphopeptides, dissociation of, ESI-FTICR-MS and IRMPD of, 121  
Arrhenius activation parameters, for loss of neutral nucleobases, 55  
Artemisinin-heme noncovalent complexes, characterization by ESI-MS and CID-MS, 1181  
Arylazido groups, photolabile, peptides modified with, MALDI-MS analysis of, 1156  
Arylglycosides, isomeric, chemical ionization of, 244  
Arylnitrenium ions, generation of, by nitro-reduction and gas phase *N*-heterocycle synthesis, 1679  
Atmospheric pressure, electrospraying water in air at, 253  
Atmospheric pressure chemical ionization (APCI). *See also* Liquid chromatography-atmospheric pressure chemical ionization.  
    in LC-MS/MS quantification of lanosterol and FF-MAS in vitro, 1216  
    of mutagenic nitropyrenes, 1853  
Atmospheric pressure chemical ionization mass spectrometry (APCI-MS)  
    charge exchange and proton transfer in, in analyzing polycyclic aromatic compounds, 301  
    gas and liquid reactions in, 311  
Atmospheric pressure photoionization (APPI)  
    in LC-MS/MS quantification of lanosterol and FF-MAS in vitro, 1216  
    of mutagenic nitropyrenes, 1853  
Atmospheric pressure photoionization mass spectrometry (APPI-MS), negative ion, 203  
Automated orthogonal control system, for ESI, 1201  
  
Bacterial spores, MALDI-TOF-MS of, 1444  
*N*-Benzoylpeptides, deprotonated, fragmentation of, 446  
Benzoxazole, DNA duplex with, ESI-MS of, 1593  
Bezimidazole, DNA duplex with, ESI-MS of, 1593  
 $\text{Bi}^{3+}$  ion, binding to transferrin, indirect detection with ESI-MS, 1658  
*Bifidobacterium lactis*, stress-related fingerprint identification from, by MALDI-TOF-MS, 1222  
Bimetallic silver-gold clusters, MALDI of, 1455  
Bioaerosol mass spectrometry (BAMS), of ionization of biomarkers from micrometer particles, 900  
Biological mass spectrometry  
    asymmetric charge partitioning in protein homodimers, 1408  
    charge competition and linear dynamic detection range in ESI-MS, 1416  
    ESI-FTICR-MS of GlcNAc-6-*O*-sulfotransferase, 1400  
    ESI mechanism features that affect protein complexes, 1424

- ESI-TOF-MS of protein kinase G, cGMP, and AMPPNP, 1392  
monomeric structures and dimer formation in  $\alpha$ -synuclein, 1435  
positive and negative ion ESI-MS of drug-DNA complexes, 1382  
Biomolecules, large, IR laser post-ionization MS of, 934  
Biopolymer ions, generated by MALDI, photodissociation of, tandem TOF MS for, 1248  
Bis-phosphate crown ethers, anionic salt bridge formation with, arginine molecular recognition by, 616  
Book reviews  
  *Encyclopedia of Mass spectrometry. Volume 1: Theory and Ion Chemistry*, 762  
  *Expanding Role of Mass Spectrometry in Biotechnology*, 625  
  *Review of the 19th Asilomar Conference on Mass Spectrometry: Bimolecular Interactions: Identification and Characterization of Protein Complexes*, 759  
Bovine serum albumin, three-dimensional structure of, chemical cross-linking and MS of, 1237  
Brain, developing, secondary ion images of, 1116  
  
C<sub>37</sub>-C<sub>40</sub> alkenones, unsaturated, double bond location in, GC-MS in derivatization for, 1161  
<sup>13</sup>C-Oleate transport, in adipocytes, multi imaging MS of, 1572  
Caffeic acid oxidation, products of, analysis by on-line EC-ESI-MS, 1228  
Calcitonins, folding analysis of, by ESI-MS with H/D exchange, 1556  
Carbon, Meisenheimer complexes bonded at, 998  
Carbon monoxide, elimination in condensation reactions in protonated dipeptides, 1025  
Carbon nanotubes, as peptide and protein affinity probes, in MALDI MS, 1629  
Carbon and nitrogen isotope ratios, in cells, 478  
Carbonyl compounds, water-solvated ammonia radical cation reactions with, 966  
Cassette dosing practices, in pharmaceutical industry, survey results on, 1374  
CD4/lc-copurifying proteins, identification with PAGE and MS, 558  
Cells, carbon and nitrogen stable isotope ratios in, 478  
Cerebellum, gangliosides from, automated nanoelectrospray MS/MS of, 1649  
Charge competition, in ESI-MS, 1416  
Charge exchange, in APCI-MS, in analyzing polycyclic aromatic compounds, 301  
Charge exchange ionization, of long-lived excited electronic states of dichloroethylene cation isomers, 1266  
Charge partitioning, asymmetric, in protein homodimers, 1408  
Chemical cross-linking, of bovine serum albumin three-dimensional structure, 1237  
Chemical ionization mass spectrometry study, of gas phase reactivity of isomeric arylglycoside toward amines, 244  
Chiral enrichment of serine, via ion soft-landing, 1360  
Chiral recognition, of zinc(II) ion complexes, by CID, 795  
Cholesterol ozonolysis, hydroperoxy bishemiacetal product derived from, ESI-MS/MS of, 194  
Chromatographic pipette tips, nano-ESI-MS/MS from, 1333  
Chronic lymphocytic leukemia, histone modifications in, HPLC and MS of, 77  
Cleavage reactions, of complex ions, positive ion ESI-MS/MS of, 689  
Collision-activated dissociation (CAD)  
  of gas phase salt complexes, stereoselectivity in, 1509  
  in quadrupole ion trap, cyclic protonated peptide and metal complex characterization by, 1039  
Collision-induced dissociation (CID). *See also* Electrospray ionization-collision-induced dissociation-tandem mass spectrometry.  
  in chiral recognition of zinc(II) ion complexes, 795  
  improved, on MALDI-TOF, 522  
  multiple-resonance, leucine enkephalin low-energy sequential decomposition pathways established in, 1794  
  of protein mixtures, 1341  
  in quadrupole TOF MS, generating protein sequence tags by, 1478  
Collisional activation  
  intermolecular migration during, monitored by H/D exchange and FTICR MS/MS, 639  
  in radio frequency ion traps and guides, 1616  
  in triple quadrupole mass spectrometer, alkenamide fragmentation by, 1462  
Collisional cooling, within the nitric oxide synthase oxygenase domain, 629  
Column switching, DNA-phosphate adduct analysis with, 593  
Composition-based sequencing, mass determination by FTICR-MS, 703  
COMSPARI (comparison of spectral retention information), in GC-MS and LC-MS of identifying minor compounds in complex mixtures, 580  
Condensation reactions, in protonated dipeptides, 1025  
Conference review, Mass spectrometry PittCon 2004, 942  
Copolymers  
  with compositional drifts or sequence constraints, mass spectra of, 374  
  isobutylene/ $\mu$ -methylstyrene, compositional analysis by MALDI-MS, 621  
Cross-ring cleavage, in glycoconjugate mixtures, 1863  
 $\alpha$ -Cyano-4-hydroxycinnamic acid clusters, MALDI-PSD and LIFT-TOF/TOF of, 336  
Cyclic GMP, ESI-TOF-MS of, 1392  
Cyclic peptides  
  IM-MS of, 870  
  protonated, MS<sup>n</sup> characterization of, 1039  
Cyclic sudden sampling introduction mode, in MIMS, 823  
Cyclopentylimino derivatization, for double bond location in polyunsaturated long chain alkenones, GC-MS in, 1161  
Cysteine-containing peptides, protonated ions of, fragmentation of, 697  
Cytochrome *c*  
  modification by 4-hydroxy-2-nonenal, 1136  
  probing structure of, by ESI-MS, 1612  
Cytosine nucleoside, self-assembling into dimers, evaluation with ESI-MS/MS, X-ray diffractometry, and theoretical calculations, 268, 436  
  
Decomposition pathways, low-energy sequential, of leucine enkephalin, using multiple-resonance CID in quadrupole ion guide, 1794  
Deoxydinucleotides, self-complementary, complex ions derived from, cleavage reactions of, positive ion ESI-MS/MS of, 689  
Deoxyribose radicals, modeling by neutralization-reionization MS, 1055, 1068  
Deuterium labeling, regiospecificity in, MS of, 1366  
Diacylene radical cation, ethylene reactions with, 114  
Dichloroethylene cation isomers, long-lived excited electronic states of, charge exchange ionization of, 1266  
Differential electrochemical mass spectrometry, 1693  
Differential electrospray emitter, potential build-up and gradient mapping within, 1737  
Dimer formation, in  $\alpha$ -synuclein, pH dependence of, monomeric structures and, 1435  
2,3-Dimethyl-2-butanol, photoionization of, 989  
Dinitropyrene, LC-MS/MS analysis of, 1853  
Dipeptides, protonated, condensation reactions in, 1025

- Dissociation, of heparin disaccharides, ion trap MS/MS of, 1274  
3,3'-Dithiobis(sulfosuccinimidyl propionate), unexpected reactivity with peptides, 736
- DNA  
  automated de novo sequencing of, by LC-MS/MS, 32  
  MS/MS sequencing of, 510  
  noncovalent interaction with peptide, MALDI-TOF detection of, 28
- DNA-bezoxazole or DNA-benzimidazole complex, ESI-MS of, 11593
- DNA cross-links, determination by MS/MS, 1565
- DNA-drug complexes, positive and negative ion ESI-MS of, 1382
- DNA-phosphate adducts, analysis with miniaturized LC-ESI-MS/MS and column switching, 593
- Droplet, single on-line, deposition for MALDI-MS, 1471
- DTSSP. *See* 3,3'-Dithiobis(sulfosuccinimidyl propionate).
- Editorials, 951, 1379, 1691
- Electrochemical mass spectrometry (EC-MS)  
  differential, 1693  
  potential build-up and gradient mapping within emitter, 1737  
  ferrocenoyl piperazide using, 1727  
  mass tags by, for protein MS, 1767  
  metabolomic applications of, 1717  
  porous flow-through electrode emitter in, 1755  
  in protein oxidation and cleavage, 1707  
  signal intensities in, ground loop current effects on, 1748
- Electrochemistry/electrospray ionization mass spectrometry (EC-ESI-MS), on-line, caffeic acid oxidation product analysis by, 1228
- Electron capture dissociation (ECD)  
  at low temperature, 1869  
  single d-amino acid distinguished in protein and tertiary structure probed by, 1087
- Electron impact conditions, MS of *O,O*-dialkyl *N,N*-dialkyl phosphoramides under, 547
- Electronic states, long-lived excited, of dichloroethylene cation isomers, charge exchange ionization of, 1266
- Electrospray. *See also* Liquid chromatography-electrospray tandem mass spectrometry.
- Electrospray emitter  
  differential, potential build-up and gradient mapping within, 1737  
  porous flow-through, analyte oxidation in electrospray ion source using, 1755
- Electrospray ion source  
  analyte oxidation in, using porous flow-through emitter, 1755  
  as chemical reactor, of anionic  $\alpha$ -adducts in gas phase, 927
- Electrospray ionization (ESI)  
  automated orthogonal control system for, 1201  
  mechanism features affecting protein complexes, 1424  
  quadrupole ion trap MS with, sulfatide studies using, 536
- Electrospray ionization-collision-induced dissociation-tandem mass spectrometry (ESI-CID-MS-MS)  
  in characterization of artemisinin-heme noncovalent complexes, 1181  
  of glycerophosphoethanolamine plasmalogen phospholipids, 1499  
  tetronasin fragmentation studies using, 325
- Electrospray ionization-time-of-flight mass spectrometry (ESI-TOF-MS), of protein kinase G, cGMP, and AMPPNP, 1392
- Electrospray ionization (ESI) conditions, proton affinity values of MALDI matrices under, estimation with kinetic method, 431
- Electrospray ionization-Fourier transform ion cyclotron resonance mass spectrometry (ESI-FTICR-MS)  
  of aromatic vs aliphatic phosphopeptide dissociation, 121  
  of GlcNAc-6-*O*-sulfotransferase, 1400
- Electrospray ionization-ion trap mass spectrometry, in discrimination of arginine dipeptide isomers, 840
- Electrospray ionization mass spectrometry (ESI-MS)  
  charge competition and linear dynamic detection range in, 1416  
  of cytochrome *c* structure, 1612  
  of DNA-bezoxazole or DNA-benzimidazole complex, 1593  
  H-D exchange combined with, in calcitonin folding analysis, 1556  
  in indirect detection of protein-metal binding, 1658  
  of leech hemoglobin subunit structure, 22  
  microfabricated nanospray tips for, nib-like design for, 407  
  multiple substrate, determination of enzyme-substrate specificity constants using, 233  
  positive and negative ion, of drug-DNA complexes, 1382  
  signal intensities in, ground loop current effects on, 1748
- Electrospray ionization-tandem mass spectrometry (ESI-MS-MS)  
  of acidic heteroxylans uronosyl substitution patterns, 43  
  of cytosine nucleosides self-assembling into dimers, 268, 436  
  of hydroperoxy bishemiacetal product derived from cholesterol ozonolysis, 194  
  medicinal herb saponin structural analysis with, 133  
  of methylarginine-containing peptide fragmentation pathways, 142  
  of mutagenic nitropyrenes, 1853  
  positive ion, of cleavage reactions of complex ions, 689  
  of *Salmonella typhimurium* acylphosphatidylglycerols, 1  
  triple quadrupole, in molecular characterization of thiols, 288
- Electrospray mass spectrometry (ESMS)  
  glycoprotein profiling by, 750  
  of 4-hydroxy-2-alkylquinolines from *Pseudomonas aeruginosa*, 862
- Electrospray time-of-flight mass spectrometry (ESMS-TOF), of  $\text{Ti}_6\text{O}_4(\text{O}_2\text{C}_4\text{H}_5)_8(\text{OCH}_2\text{CH}_3)_8$ , 260
- Electrospraying, of water in air at atmospheric pressure, 253
- Emitter, electrospray, potential build-up and gradient mapping within, 1737
- Enolic radical cations, 1,3-H shifts of, orbital symmetry restraint circumvention by, 972
- Enzymatic digestion studies, of advanced glycation end products-peptides, 496
- Enzyme-substrate specificity constants, determination using multiple substrate ESI-MS assay, 233
- Epoxides, Meerwein reaction of phosphonium ions with, in gas phase, 398
- Ethanol, hydrogen atom abstraction from, phenyl radical selectivity in, 913
- Ethyl sulfate, forensic confirmatory analysis of, by LC-ESI-MS-MS, 1644
- Ethylene, diacetylene radical cation reactions with, 114
- Ethylglucuronide, in urine, LC-ESI-MS-MS of, 188
- Ferrocenoyl piperazide, using LC-EC-S, 1727
- FF-MAS, quantification by LC-APPI-MS-MS in vitro, 1216
- Field asymmetric waveform ion mobility spectrometry (FAIMS), modeling resolution and sensitivity of, 1487
- Flavonoids  
  determining glycosylation site of, by metal complexation and MS-MS, 1287  
  gas phase acidities of, 848
- Folding analysis, of calcitonins, by ESI-MS with H-D exchange, 1556
- Formic acid, protonated, decomposition of, 982

- Fourier transform ion cyclotron resonance (FTICR). *See also* Electrospray ionization-FTICR; Liquid chromatography-FTICR.
- Fourier transform ion cyclotron resonance (FTICR) mass spectrometry, in composition-based sequencing of peptides, mass determination by, 703
- Fourier transform ion cyclotron resonance (FTICR) tandem mass spectrometry, H-D exchange integration with, in monitoring intermolecular migration during collisional activation, 639
- Fourier transform mass spectrometry (FTMS)  
for large targets with diverse surfaces, MALDI ion source for, 128  
peak position determination in, 457
- Fragmentation  
of ACE inhibitors, MS in, 1300  
of alkenamides, by collisional activation in triple quadrupole mass spectrometer, 1462  
of amidinated peptide ions, 158  
competing processes of, in MS-MS of heparin-like glycosaminoglycans, 1534  
of deprotonated *N*-benzoylpeptides, 446  
of glycosidic bonds, in gas phase, direction by non-covalent complexes, 715  
of protonated ions of cysteine-containing peptides, 697  
of protonated oligoalanines, 1810  
of tetronasin, ESI-CID-MS-MS studies of, 325
- Fragmentation pathways, in methylarginine-containing peptides, ESI-MS-MS of, 142
- Free fatty acid transport, in adipocytes, multi imaging MS of, 1572
- Gangliosides, cerebellar, automated nanoelectrospray MS-MS of, 1649
- Gas chromatography Fourier transform mass spectrometry (GC-FTMS), preconstructor coupled to, 1191
- Gas chromatography mass spectrometry (GC-MS)  
in identifying minor compounds in complex mixtures, COMSPARI and, 580  
of neuromelanin pyrolysis products, 920  
in phenyl- and cyclopentylimino derivatization for double bond location in unsaturated C<sub>37</sub>-C<sub>40</sub> alkenones, 1161
- Gas phase  
anionic  $\alpha$ -adducts in, using electrospray ion source as chemical reactor, 927  
flavonoid acidities in, 848  
glycosidic bond fragmentation in, direction by non-covalent complexes, 715  
gramicidin S and linear analog conformational preferences in, IM-MS of, 870  
halide S<sub>N</sub>2 reactions with halodimethylamine in, 673  
ion chemistry of methylbenz(is)oxazole isomers in, 1005  
isomeric arylglycoside reactivity toward amines in, 244  
loss of nucleobases from deprotonated oligonucleotide anions in, Arrhenius activation parameters for, 55  
Meerwein reaction of phosphonium ions with epoxides and thioepoxides in, 398  
Meisenheimer complexes bonded in, 998  
*N*-heterocycle synthesis in, in arylnitrenium ion generation, 1679  
Ni(II) complex reactions with acetonitrile, 1128  
oligonucleotide duplexes in, stability determination of, 1354  
paralytic shellfish poison behavior in, 462  
peptide acidity from adduct dissociation in, 616  
protonated tryptophan reactions in, 65  
salt complexes in, CAD of, stereoselectivity in, 1509  
sodiated peptide formation in, 607  
solvation of propanediol ions by water molecules in, 1123  
thiol and thioester nitrosation in, 344
- Gas reactions, in APCI-MS sources, 311
- Genotyping, semi-quantitative, of single nucleotide polymorphisms, LC-MS for, 1897
- GlcNAc-6-*O*-sulfotransferase, ESI-FTICR-MS of, 1400
- Glycerophosphoethanolamine plasmalogen phospholipids, ESI-MS/MS of, 1499
- Glycoconjugate mixtures, cross-ring cleavage in, 1863
- Glycopeptides, gp120, from HIV, LC-MS of, 1545
- Glycoproteins  
analysis of, Q-trap mass spectrometer in, 413  
electrospray MS profiling of, 750
- Glycosaminoglycans, heparin-like, MS/MS of, competing fragmentation processes in, 1534
- Glycosidic bond fragmentation, in gas phase, direction by non-covalent complexes, 715
- Glycosylation site, of flavonoids, determining by metal complexation and MS/MS, 1287
- Gold-silver clusters, bimetallic, MALDI of, 1455
- gp120 glycopeptides, from HIV, LC-MS of, 1545
- Gramicidin S and linear analogs, conformational preferences in gas phase, IM-MS of, 870
- Ground loop current, signal intensities and, in ESI-MS, 1748
- Halides, S<sub>N</sub>2 reactions with halodimethylamine, in gas phase, 673
- Halodimethylamine, halide S<sub>N</sub>2 reactions with, in gas phase, 673
- Heme-artemisinin noncovalent complexes, characterization by ESI-MS and CID-MS, 1181
- Hemoglobin, from leech, subunit structure of, ESI-MS of, 22
- Heparin disaccharides, dissociation mechanisms of, ion trap MS/MS of, 1274
- Heparin-like glycosaminoglycans, MS/MS of, competing fragmentation processes in, 1534
- Herbicides, rearrangement reactions of, in MALDI-FTMS, 1820
- Herbs, medicinal, saponins from, ESI-MS/MS structural analysis of, 133
- N*-Heterocycle synthesis, in gas phase, in arylnitrenium ion generation, 1679
- Heteroxylans, acidic, uronosyl substitution patterns in, ESI-MS/MS of, 43
- High pressure liquid chromatography (HPLC), of histone modifications in leukemia, 77
- High throughput screening, for binding to RNA, 884
- Histidine adducts, in cytochrome *c* modification by 4-hydroxy-2-nonenal, 1136
- Histone, modifications in leukemia, HPLC and MS of, 77
- Hop extract, bitter acids from, LC-APCI-MS of, 180
- Human immunodeficiency virus (HIV), gp120 glycopeptides from, LC-MS of, 1545
- Hydration, intrinsic, of monocationic uranyl hydroxide, nitrate, and acetate cations, 777
- Hydrogen atom, abstraction from ethanol, phenyl radical selectivity in, 913
- Hydrogen/deuterium exchange  
amide, modeling data from, in protein-ligand interactions, 388  
ESI-MS with, in calcitonin folding analysis, 1556
- Hydrogen deuterium exchange, FTICR MS/MS integration with, in monitoring intermolecular migration during collisional activation, 639
- Hydroperoxy bishemiacetal product, derived from cholesterol ozonolysis, ESI-MS/MS of, 194
- 4-Hydroxy-2-alkylquinolines, from *Pseudomonas aeruginosa*, ESI-LC-MS of, 862
- 4-Hydroxy-2-nonenal, cytochrome *c* modification by, 1136



- 2-Hydroxyoxolan-2-yl radical, modeling by neutralization-reionization MS, 1055
- 3-Hydroxyoxolan-3-yl radical, modeling by neutralization-reionization MS, 1068
- Imaging, secondary ion, of developing brain, 1116
- $\text{In}^{3+}$  ion, binding to transferrin, indirect detection with ESI-MS, 1658
- Inductively coupled plasma mass spectrometry (ICP-MS), laser ablation for, 769
- Infrared laser post-ionization mass spectrometry, of large biomolecules, 934
- Infrared multiphoton dissociation (IRMPD)  
of aromatic vs aliphatic phosphopeptide dissociation, 121  
of phosphopeptides, 1581
- Intrinsic hydration, of monocationic uranyl hydroxide, nitrate, and acetate cations, 777
- Ion  
complex, cleavage reactions of, positive ion ESI-MS/MS of, 689  
metastable, 1261  
protonated, of cysteine-containing peptides, fragmentation of, 697
- Ion chemistry, of methylbenz(is)oxazole isomers in gas phase, 1005
- Ion energy, in quadrupole MS, 48
- Ion mobility, high-field, resolution equations for, 1320
- Ion mobility mass spectrometry, applied to cyclic peptide analysis, 870
- Ion soft-landing  
chiral enrichment of serine via, 1360  
into liquids, 1874
- Ion source, for medium pressure laser ionization, 1885
- Ion trap-ion mobility-time-of-flight mass spectrometer, nano-flow LC with, to analyze protein mixtures, 1341
- Ion trap, radio frequency, collisional activation in, 1616
- Ion trap tandem mass spectrometry  
data-dependent, in proteomics, 150  
of heparin disaccharide dissociation mechanisms, 1274
- Ionic-liquid matrices, for quantitative analysis by MALDI-TOF-MS, 1833
- Ionization  
medium pressure laser, ion source for, 1885  
soft, of organic compounds, PERCI for, 424
- Isobaric interferences, deconvolution of, in mass spectra, 654
- Isobutylene/ $\mu$ -methylstyrene copolymers, compositional analysis by MALDI-MS, 621
- Isotope labeling, in phosphopeptide quantification, 363
- Isotopic peaks, isotopic composition and accurate masses of, 12
- Kinetic method  
in determining proton affinity of nucleic acid molecules, 1080  
in discrimination of arginine dipeptide isomers, 840  
in estimating proton affinity values of MALDI matrices under ESI conditions, 431
- Lanosterol, quantification by LC-APPI-MS/MS in vitro, 1216
- Laser ablation, for ICP-MS, 769
- Laser ionization, medium pressure, ion source for, 1885
- Leech, hemoglobin from, subunit structure of, ESI-MS of, 22
- Letter to the editor, on computer software to calculate weight in Daltons of ions, 626
- Leucine enkephalin, low-energy sequential decomposition pathways of, using multiple-resonance CID in quadrupolar ion guide, 1794
- Leukemia, acute myeloid and chronic lymphocytic, histone modifications in, HPLC and MS of, 77
- LIFT-TOF/TOF, of CHCA clusters, 336
- Linear dynamic detection range, in ESI-MS, 1416
- Lipid chemistry, MALDI-FTMS of, strategy and data analysis techniques for, 1665
- Liquid(s), ion soft-landing into, 1874
- Liquid chromatography-atmospheric pressure chemical ionization mass spectrometry (LC-APCI-MS)  
of bitter acids in crude hop extract, 180  
of mutagenic nitropyrenes, 1853
- Liquid chromatography-atmospheric pressure photoionization-tandem mass spectrometry (LC-APPI-MS/MS)  
lanosterol and FF-MAS quantification by, in vitro, 1216  
of mutagenic nitropyrenes, 1853
- Liquid chromatography-electrochemical mass spectrometry (LC-EC-MS), ferrocenoyl piperazide using, 1727
- Liquid chromatography-electrospray ionization-tandem mass spectrometry (LC-ESI-MS/MS)  
of ethyl sulfate as marker of alcohol consumption, 1644  
of ethylglucuronide in urine, 188  
miniaturized, DNA-phosphate adduct analysis with, 593
- Liquid chromatography-electrospray mass spectrometry (LC-ES-MS), negative ion, neutral O-linked oligosaccharide alditol structural determination by, 659
- Liquid chromatography-electrospray tandem mass spectrometry (LC-ES-MS/MS), miniaturized, of melphalan-modified 2'-oligodeoxynucleotides, 568
- Liquid chromatography-Fourier transform ion cyclotron resonance (LC-FTICR), for proteomics, 212
- Liquid chromatography mass spectrometry (LC-MS)  
of HIV gp120 glycopeptides, 1545  
of 4-hydroxy-2-alkylquinolines from *Pseudomonas aeruginosa*, 862  
in identifying minor compounds in complex mixtures, COMSPARI and, 580  
in semi-quantitative genotyping of single nucleotide polymorphisms, 1897
- Liquid chromatography-matrix-assisted laser desorption/ionization-time-of-flight/time-of-flight (LC-MALDI-TOF/TOF), in protein complex analysis, 803
- Liquid chromatography-tandem mass spectrometry (LC-MS/MS)  
in automated de novo DNA sequencing, 32  
lanosterol and FF-MAS quantification by, in vitro, 1216  
of N-terminal phospholipase A<sub>2</sub> processing and amyloid precursor protein potential cleavage sites, 1780
- Liquid reactions, in APCI-MS sources, 311
- Lithiated valine, water binding energies to, 1014
- Lymphocytic leukemia, chronic, histone modifications in, HPLC and MS of, 77
- Lysine, chemical cross-linking with tyrosine, 1604
- Lysine adducts, in cytochrome c modification by 4-hydroxy-2-nonenal, 1136
- $[\text{M} + \text{H}]^+$  formation, mechanism of, in photoionization MS, 1521
- Macromolecule mass spectrometry, citation mining of user documents in, 281
- Mass spectra  
of alkyl diselenide and selenosulfenate, 1325  
of copolymers with compositional drifts or sequence constraints, 374  
deconvolution of isobaric interferences in, 654  
high resolution, new matching algorithm for, 1173  
normalization of, 385
- Mass spectrometer, triple quadrupole, collisional activation in, alkenamide fragmentation by, 1462
- Mass spectrometry (MS)  
in ACE inhibitor fragmentation, 1300

- of advanced glycation end products/peptides, 496
- of bovine serum albumin three-dimensional structure, 1237
- of CD4/lc-copurifying proteins, 558
- in detection of affinity purified cross-linked peptides, 832
- of deuterium labeling regiospecificity, 1366
- electrochemistry combined with. *See* Electrochemical mass spectrometry.
- of histone modifications in leukemia, 77
- modeling data from, in protein-ligand interactions, 388
- multi imaging, of  $^{13}\text{C}$ -oleate transport in adipocytes, 1572
- of *O,O*-dialkyl *N,N*-dialkyl phosphoramides under electron impact conditions, 547
- of protein
  - improved sample processing time and peptide recovery for, 784
  - inherent electrochemistry of electrospray for, mass tag generation by, 1767
- Mass tags, by inherent electrochemistry of ESI, 1767
- Matrix-assisted laser desorption/ionization (MALDI)
  - of bimetallic silver-gold clusters, 1455
  - biopolymer ions generated by, photodissociation of, tandem TOF MS for, 1248
  - for FTMS to accommodate large targets, 128
  - in polyaniline oligomers analysis, 893
- Matrix-assisted laser desorption/ionization Fourier transform mass spectrometry (MALDI-FTMS)
  - herbicide rearrangements in, 1820
  - lipid and phospholipid chemistry elucidation by, strategy and data analysis techniques for, 1665
- Matrix-assisted laser desorption/ionization (MALDI) mass spectrometry
  - in analysis of photolabile peptides, 1156
  - carbon nanotubes as affinity tubes for peptides and proteins in, 1629
  - isobutylene/ $\mu$ -methylstyrene copolymer compositional analysis by, 621
  - on-line single droplet deposition for, 1471
  - polymer, sample deposition for, 168
  - simple organic molecule cationization in, 879
- Matrix-assisted laser desorption/ionization (MALDI) matrices
  - liquid based UV, detection limits of proteins from, 486
  - proton affinity values of, under ESI conditions with kinetic method, 431
- Matrix-assisted laser desorption/ionization post-source decay (MALDI-PSD), of CHCA clusters, 336
- Matrix-assisted laser desorption/ionization tandem mass spectrometry-post-source decay (MALDI-MS/MS-PSD), of phenylhydrazone-oligosaccharides from ovalbumin, 725
- Matrix-assisted laser desorption/ionization tandem time-of-flight (MALDI-TOF/TOF) mass spectrometry, of *N*-sulfonated peptides, 1838
- Matrix-assisted laser desorption/ionization time-of-flight (MALDI-TOF) mass spectrometry
  - of bacterial spores, 1444
  - improved PSD and CID on, 522
  - noncovalent peptide-DNA interaction detected with, 28
  - quantitative analysis by, ionic-liquid matrices for, 1833
  - in stress-related fingerprint identification from *Bifidobacterium lactis*, 1222
- McLafferty rearrangement, 951, 956
  - binding energies of water to lithiated valine, 1014
  - within a complex, 966
  - condensation reactions in protonated dipeptides, 1025
  - construction of hybrid quadrupole FTICR-MS, for MS/MS, 1099
  - decomposition of protonated formic acid, 982
  - ECD distinguishing single d-amino acid in, 1087
- Meisenheimer complexes bonded in gas phase, 998
- modeling deoxyribose radicals by neutralization-reionization MS, 1055, 1068
- MS/MS of methylbenz(is)oxazole isomers, 1005
- $\text{MS}^n$  characterization of protonated cyclic peptides and metal complexes, 1039
- orbital symmetry restraint circumvention in, 972
- photoionization of hexyl alcohol, 989
- proton affinity of nucleic acid molecules, kinetic method in, 1080
- in secondary ion images of developing brain, 1116
- solution equivalent of, 959
- Medicinal herbs, saponins from, ESI-MS/MS structural analysis of, 133
- Medium pressure laser ionization, ion source for, 1885
- Meerwein reaction, of phosphonium ions with epoxides and thioepoxides in gas phase, 398
- Meisenheimer complexes, bonded in gas phase, 998
- Melphalan-modified 2'-oligodeoxynucleotides, miniaturized LC-ES MS/MS of, 568
- Membrane inlet mass spectrometry (MIMS), cyclic sudden sampling introduction mode in, 823
- Metabolomics, EC-MS in, 1717
- Metal clusters, molecule interactions with, MALDI-MS of, 879
- Metal complexation, flavonoid glycosylation site determination by, 1287
- Metal complexes,  $\text{MS}^n$  characterization of, 1039
- Metal trications, attachment to peptides, 406
- Metastable atom bombardment ionization mass spectrometry (MAB-MS), for identifying additives in polymers, 1315
- Metastable ions, half-protons or doubly charged ions as, 1261
- Methylarginine-containing peptides, fragmentation pathways in, ESI-MS/MS of, 142
- Methylbenz(is)oxazole isomers, MS/MS of, 1005
- Micrometer particles, ionization of biomarkers from, BAMS in, 900
- Modeling data, in protein-ligand interactions, 388
- Molecular energetics, temporal and spatial variations in, in millisecond pulsed radio frequency glow discharge-TOF-MS, 87
- $\text{MS}^n$  cyclic protonated peptide and metal complex characterization by, 1039
- Multi imaging mass spectrometry, of  $^{13}\text{C}$ -oleate transport in adipocytes, 1572
- Myeloid leukemia, acute, histone modifications in, HPLC and MS of, 77
- N*-benzoylpeptides, deprotonated, fragmentation of, 446
- N*-heterocycle synthesis, in gas phase, in arylnitrenium ion generation, 1679
- N*-terminal processing, of phospholipase  $\text{A}_2$ , LC-MS/MS of, 1780
- Nanoelectrospray ionization tandem mass spectrometry (nano-ESI-MS/MS)
  - automated, of cerebellar gangliosides, 1649
  - from chromatographic pipette tips, 1333
- Nanoflow liquid chromatography-ion mobility mass spectrometry, of protein mixtures, 1341
- Nanospray tips, microfabricated, nib-like design for, 407
- Negative ion atmospheric pressure photoionization mass spectrometry (APPI-MS), 203
- Negative ion liquid chromatography-electrospray mass spectrometry, neutral *O*-linked oligosaccharide alditol structural determination by, 659
- Neosaitoxin, protonated, gas phase dissociation reactions of, 462
- Nephelopsis obscura*, hemoglobin from, subunit structure of, ESI-MS of, 22

- Neuromelanin, pyrolysis products of, from substantia nigra, GC-MS analysis of, 920
- Neutralization-reionization MS, modeling deoxyribose radicals by, 1055, 1068
- Nickel complex ions, reactions with acetonitrile in gas phase, 1128
- Nitrate-anion complex, monopositive, intrinsic hydration of, 777
- Nitric oxide synthase oxygenase domain, collisional cooling within, 629
- Nitro-reduction, in arylnitrenium ion generation, 1679
- Nitrogen isotopes, carbon isotope ratios to, in cells, 478
- Nitropyrenes, mutagenic, LC-MS/MS analysis of, 1853
- Nitrosation, of thiols and thioesters, in gas phase, 344
- Non-covalent complexes, in glycosidic bond fragmentation in gas phase, 715
- Nucleic acid molecules, proton affinity of, kinetic method determination of, 1080
- Nucleobases, loss of, Arrhenius activation parameters for, 55
- Nucleosides, cytosine, self-assembling into dimers, evaluation with ESI-MS/MS, X-ray diffractometry, and theoretical calculations, 268, 436
- $^{16}\text{O}/^{18}\text{O}$  peptide ion ratio, calculating for proteome relative quantification, 437
- Obituaries  
Isamu Matsumoto, 1689  
Andrew Gans "Jack" Sharkey, Jr., 627  
Victor L. Talroze, 1517
- $^{13}\text{C}$ -Oleate transport, in adipocytes, multi imaging MS of, 1572
- Oligoalanines, protonated, fragmentation of, 1810
- 2'-Oligodeoxynucleotides, melphalan-modified, miniaturized LC-ES MS/MS of, 568
- Oligomers, polyaniline, MALDI analysis of, 893
- Oligonucleotide, DNA sequencing of, by MS/MS, 510
- Oligonucleotide anions, deprotonated, loss of nucleobases from, Arrhenius activation parameters for, 55
- Oligonucleotide duplexes, stability determination of, in gas and solution phase, 1354
- Oligopeptides, protonated, MS/MS of, amide bond cleavage mechanism in, 103
- Oligosaccharide alditols, neutral O-linked, structural determination by negative ion LC-ESI-MS, 659
- Oligosaccharides, from ovalbumin, phenylhydrazones of, MALDI-MS/MS-PSD of, 725
- On-line single droplet deposition, for MALDI-MS, 1471
- O,O-dialkyl N,N-dialkyl phosphoramides, MS of, under electron impact conditions, 547
- Orbital symmetry restraint circumvention, by 1,3-H shifts of enolic radical cations, 972
- Organic compounds, soft ionization of, PERCI for, 424
- Organic molecules, simple, cationization of, in MALDI-MS, 879
- Orthogonal control system, automated, for ESI, 1201
- Ovalbumin, phenylhydrazone-oligosaccharides from, MALDI-MS/MS-PSD fragmentation study of, 725
- Oxazolones, deprotonated, formation of, 446
- Oxidation, of analyte, in electrospray ion source using porous flow-through emitter, 1755
- Oxygen, Meisenheimer complexes bonded at, 998
- Paclitaxel, ionization and adduct formation of, 585
- Paralytic shellfish poisons, gas phase dissociation reactions of, 462
- Peptide(s)  
affinity purified cross-linked, MS detection of, 832  
assigning to tandem mass spectra, SILVER in, 910  
carbon nanotubes as affinity tubes for, in MALDI MS, 1629  
composition-based sequencing of, mass determination by FTICR-MS, 703  
cyclic, IM-MS of, 870  
cyclic protonated,  $\text{MS}^n$  characterization of, 1039  
cysteine-containing, protonated ions of, fragmentation of, 697  
DTSSP unexpected reactivity with, 736  
metal trication attachment to, 406  
methylarginine-containing, fragmentation pathways in, ESI-MS/MS of, 142  
modified with photolabile arylazido groups, MALDI-MS analysis of, 1156  
N-sulfonated, MALDI-TOF/TOF-MS of, 1838  
noncovalent interaction with DNA, MALDI-TOF detection of, 28  
protonated, condensation reactions in, 1025  
sodiated, formation in gas phase, 607
- Peptide ion ratio,  $^{16}\text{O}/^{18}\text{O}$ , calculating for proteome relative quantification, 437
- Peptide ions, amidinated, fragmentation of, 158
- Peptide recovery, in MS of protein digests, 784
- pH,  $\alpha$ -synuclein dimer formation dependence on, monomeric structures and, 1435
- Pharmaceutical industry, cassette dosing practices in, survey results on, 1374
- Phenyl radical selectivity, in hydrogen atom abstraction from ethanol, 913
- Phenylhydrazone-oligosaccharides, from ovalbumin, MALDI-MS/MS-PSD fragmentation study of, 725
- Phenylimino derivatization, for double bond location in polyunsaturated long chain alkenones, 1161
- Phospholipase  $\text{A}_2$ , N-terminal processing of, LC-MS/MS of, 1780
- Phospholipid(s), glycerophosphoethanolamine plasmalogen, ESI-CID-MS/MS of, 1499
- Phospholipid chemistry, MALDI-FTMS of, strategy and data analysis techniques for, 1665
- Phosphonium ions, Meerwein reaction with epoxides and thioepoxides, in gas phase, 398
- Phosphopeptides  
aromatic vs aliphatic, dissociation of, ESI-FTICR-MS and IRMPD of, 121  
IRMPD of, 1581  
quantification with affinity chromatography and stable isotope labeling, 363
- Photodissociation, of biopolymer ions generated by MALDI, tandem TOF MS for, 1248
- Photoelectron resonance capture ionization (PERCI), for soft ionization of organic compounds, 424
- Photoionization, of hexyl alcohol, 989
- Photoionization mass spectrometry, mechanism of  $[\text{M} + \text{H}]^+$  formation in, 1521
- Photolabile arylazido groups, peptides modified with, MALDI-MS analysis of, 1156
- Pipette tips, chromatographic, nano-ESI-MS/MS from, 1333
- Pivaloyl cation, carbocationic rearrangement of, 959
- Polyacrylamide gel electrophoresis, of CD4/lc-copurifying proteins, 558
- Polyaniline oligomers, MALDI analysis of, 893
- Polycyclic aromatic compounds, analysis with APCI-MS, charge exchange and proton transfer in, 301
- Polymer  
identifying additives in, TPPy/MAB-MS for, 1315  
MALDI-MS of, sample deposition for, 168
- Polymorphisms, single nucleotide, semi-quantitative genotyping of, LC-MS for, 1897
- Positive ion electrospray ionization-tandem mass spectrometry, of cleavage reactions of complex ions, 689

- Positive ion mass spectra, from APCI-MS gases and solvents used in LC and direct liquid injection, 311
- Post-ionization separations, FAIMS in, modeling resolution and sensitivity of, 1487
- Post-source decay (PSD), improved, on MALDI-TOF, 522
- Potential build-up and gradient mapping, in differential electrospray emitter, 1737
- Preconstructor, GC-FTMS coupled to, 1191
- Propanediol ions, solvation by water molecules in gas phase, 1123
- Protein(s)
- carbon nanotubes as affinity tubes for, in MALDI MS, 1629
  - CD4/lc-copurifying, PAGE and MS of, 558
  - chemical cross-linking of, 1604
  - electrochemical oxidation and cleavage of, 1707
  - from liquid based UV-MALDI matrices, detection limits of, 486
  - single d-amino acid distinguished in, by ECD, 1087
- Protein complexes
- ESI mechanism features affecting, 1424
  - LC-MALDI-TOF/TOF analysis of, 803
- Protein digests, MS of, improved sample processing time and peptide recovery for, 784
- Protein glycosylation, analysis with Q-trap mass spectrometer, 413
- Protein homodimers, asymmetric charge partitioning in, 1408
- Protein kinase G, ESI-TOF-MS of, 1392
- Protein-ligand interactions, modeling data in, 388
- Protein mass spectrometry, inherent electrochemistry of electrospray for, mass tag generation by, 1767
- Protein-metal binding, indirect detection of, ESI-MS in, 1658
- Protein mixtures, nanoflow LC-IMS-MS and LC-IMS-CID MS of, 1341
- Protein phosphorylation, stoichiometry of, 647
- Protein sequence tags, generating using CID in quadrupole TOF MS, 1478
- Proteomes, relative quantification of, calculating  $^{16}\text{O}/^{18}\text{O}$  peptide ion ratio for, 437
- Proteomics
- high performance LC-FTICR mass spectrometer for, 212
  - ion trap data-dependent MS/MS in, 150
- Proton affinity, of nucleic acid molecules, kinetic method determination of, 1080
- Proton affinity values, of MALDI matrices under ESI conditions with kinetic method, 431
- Proton transfer, in APCI-MS, in analyzing polycyclic aromatic compounds, 301
- Protonated dipeptides, condensation reactions in, 1025
- Protonated formic acid, decomposition of, 982
- Protonated ions, of cysteine-containing peptides, fragmentation of, 697
- Protonated peptides, cyclic,  $\text{MS}^n$  characterization of, 1039
- Protons, half or doubly charged, metastable ions as, 1261
- Pseudomonas aeruginosa*, 4-hydroxy-2-alkylquinolines from, ESI-LC-MS of, 862
- Q-trap mass spectrometer, in glycoprotein analysis, 413
- Quadrupole/Fourier transform ion cyclotron resonance mass spectrometer, construction of, for MS/MS, 1099
- Quadrupole ion trap, CAD in, cyclic protonated peptide and metal complex characterization by, 1039
- Quadrupole ion trap mass spectrometry, ESI with, sulfatide studies using, 536
- Quadrupole mass spectrometer, triple, collisional activation in, alkenamide fragmentation by, 1462
- Quadrupole mass spectrometry, ion energy in, 48
- Quadrupole tandem mass spectrometry (MS/MS), triple, in molecular characterization of thiols, 288
- Quadrupole time-of-flight mass spectrometer, CID in, generating protein sequence tags by, 1478
- Radio frequency glow discharge-time of flight mass spectrometry, millisecond pulsed, temporal and spatial variations in molecular energetics, 87
- Radio frequency ion traps and guides, collisional activation in, 1616
- Resolution equations, for high-field ion mobility, 1320
- RNA, binding to, high throughput screening for, 884
- Robinson, Carol V., 2003 Biemann Medal awardee, 1379
- Salmonella typhimurium*, acylphosphatidylglycerols from, ESI-MS/MS of, 1
- Salt, anionic, in arginine molecular recognition, 616
- Salt complexes, in gas phase, CAD of, stereoselectivity in, 1509
- Sample deposition, for polymer MALDI-MS, 168
- Sample processing time, in MS of protein digests, 784
- Saponins, from medicinal herbs, ESI-MS/MS structural analysis of, 133
- Saxitonix, protonated, gas phase dissociation reactions of, 462
- Selenosulfenate, mass spectra of, 1325
- Self-complementary deoxydinucleotides, complex ions derived from, cleavage reactions of, positive ion ESI-MS/MS of, 689
- Serine, chiral enrichment of, via ion soft-landing, 1360
- SIFT ion-molecule study, of reactions in Titan's atmosphere, 1148
- SILVER, in assigning peptides to tandem mass spectra using intensity-based scoring, 910
- Silver-gold clusters, bimetallic, MALDI of, 1455
- Sodium cationized peptides, formation in gas phase, 607
- Solution phase
- oligonucleotide duplexes in, stability determination of, 1354
  - structure of, water binding energies to lithiated valine in, 1014
- Spider venom acylpolyamides, MS/MS of, 1636
- Spores, bacterial, MALDI-TOF-MS of, 1444
- Stereoselectivity, in CAD of gas phase salt complexes, 1509
- Stress-related fingerprint identification, from *Bifidobacterium lactis*, by MALDI-TOF-MS, 1222
- Substantia nigra, neuromelanin from, GC-MS analysis of, 920
- Sudden sampling introduction mode, cyclic, in MIMS, 823
- Sulfatides, quadrupole ion trap MS with ESI of, 536
- Sulfonated peptides, MALDI-TOF/TOF-MS of, 1838
- Supercid medium, carbocationic rearrangement of pivaloyl cation and protonated pivalaldehyde in, 959
- $\alpha$ -Synuclein, monomeric structures and pH-dependent dimer formation in, 1435
- Tandem mass spectra, assigning peptides to, SILVER in, 910
- Tandem mass spectrometry (MS/MS)
- construction of quadrupole-FTICR-MS for, 1099
  - in DNA cross-link determination, 1565
  - DNA sequencing by, 510
  - flavonoid glycosylation site determination by, 1287
  - of gas phase reactivity of isomeric arylglycoside toward amines, 244
  - of heparin-like glycosaminoglycans, competing fragmentation processes in, 1534
  - ion trap data-dependent, in proteomics, 150
  - of methylbenz(is)oxazole isomers, 1005
  - of protonated oligopeptides, amide bond cleavage mechanism in, 103
  - of spider venom acylpolyamides, 1636
  - triple quadrupole, in molecular characterization of thiols, 288



- Tandem time-of-flight mass spectrometer, for photodissociation of biopolymer ions generated by MALDI, 1248
- Temperature, low, ECD at, 1869
- Temperature-programmed pyrolysis/metastable atom bombardment ionization mass spectrometry (TPPy/MAB-MS), for identifying additives in polymers, 1315
- Tetronasin, ESI-CID-MS/MS fragmentation studies of, 325
- Thexyl alcohol, photoionization of, 989
- Thioepoxides, Meerwein reaction of phosphonium ions with, in gas phase, 398
- Thioesters, nitrosation in gas phase, 344
- Thiol(s)
- molecular characterization of, ESI and triple quadrupole MS/MS in, 288
  - nitrosation in gas phase, 344
- Tingle compounds, fragmentation of, by collisional activation in triple quadrupole mass spectrometer, 1462
- Ti<sub>6</sub>O<sub>4</sub>(O<sub>2</sub>C<sub>4</sub>H<sub>5</sub>)<sub>8</sub>(OCH<sub>2</sub>CH<sub>3</sub>)<sub>8</sub>, ESMS-TOF of, 260
- Titan's atmosphere, SIFT ion-molecule study of reactions in, 1148
- Titration, modeling data from, in protein-ligand interactions, 388
- Trace element analysis, laser ablation ICP-MS in, 769
- Transferrin, In<sup>3+</sup> and Bi<sup>3+</sup> binding to, indirect detection with ESI-MS, 1658
- Triple quadrupole mass spectrometer, collisional activation in, alkenamide fragmentation by, 1462
- Triple quadrupole tandem mass spectrometry (MS/MS), in molecular characterization of thiols, 288
- Tryptophan, protonated, gas phase reactions of, 65
- Tyrosine, chemical cross-linking with lysine, 1604
- Ultraviolet-MALDI matrices, liquid based, detection limits of proteins from, 486
- Uranyl hydroxide-anion complex, monopositive, intrinsic hydration of, 777
- Urine, ethylglucuronide in, LC-ESI-MS/MS of, 188
- Uronosyl substitution patterns, in acidic heteroxylans, ESI-MS/MS of, 43
- Valine, lithiated, water binding energies to, 1014
- Water
- binding energies to lithiated valine, 1014
  - electrospraying in air, at atmospheric pressure, 253
  - elimination in condensation reactions in protonated dipeptides, 1025
- Water molecules, propanediol ion solvation by, in gas phase, 1123
- Water-solvated ammonia radical cation, reactions with carbonyl compounds, 966
- X-ray diffractometry, of cytosine nucleosides self-assembling into dimers, 268, 436
- Zinc(II) ion complexes, chiral recognition of, by CID, 795